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Comment on Free-free opacity in warm aluminum by Vinko et al

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High Energy Density Physics

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Abstract

Calculations of the photon absorption in solid density aluminum by Vinko *et al* [*HEDP* 5(2009), 124-131] contain an inconsistent implementation of the pseudo-potential approach. It is shown that this inconsistency may be partially responsible for the claimed improved agreement of their model including particle-hole interactions with the experimental data for cold aluminum.

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Recently Vinko *et al* [1] presented photon absorption calculations for solid density aluminum. Briefly, their semi-analytical calculations are based on Ron and Tzoar [2], which is a weak-scattering approximation corrected for stimulated emission with a thermal average that accounts for electron degeneracy [3]. Their calculations used the empty-core electron-ion interaction screened by the random phase approximation (RPA) or local field corrected (LFC) dielectric function plus an ion structure factor for the crystal or one suitable for liquids.

The Vinko *et al* results were compared to absorption measurements in cold, solid density aluminum [1,3]. The comparisons showed that their molecular dynamics (MD) simulations agree with the cold experimental data only at low frequencies. The semi-analytic RPA model and MD calculations agree for photon energies $\hbar\omega \geq 15eV$ (lower limit of semi-analytical calculations) and there is improvement compared to the measurements with their LFC semi-analytic results. The purpose here is to note an inconsistent treatment of the pseudo-potential approach by Vinko *et al* that could compromise their claimed improved agreement with the cold data using the LFC dielectric function.

The electron-ion interaction in the Vinko *et al* semi-analytic model is the empty-core potential with Fourier transform

$$\tilde{V}(q;R_c) = -\frac{4\pi Ze^2}{q^2}\cos(qR_c) \tag{1}$$

where R_c is a free parameter constrained by fitting Fermi surface eigenvalues [1]. Interestingly, the value for R_c can vary by about a factor of 2 depending on the fitted physical quantity [4]. Nevertheless, neither the sensitivity of the absorption to R_c nor the choice of constraining experimental data was discussed by Vinko *et al*.

More importantly, there is reason for skepticism regarding the improved agreement between the cold Al experimental data and their semi-analytical LFC calculations. Specifically, the statically screened pseudo-potential,

$$\tilde{V}_s(q;R_c) = \frac{\tilde{V}(q;R_c)}{\varepsilon(q,0)} \tag{2}$$

with $\varepsilon(q,\omega)$ the free-electron gas dielectric function is used to determine R_c [4]. Vinko *et al*, however, used $R_c = 0.6\text{Å}$ in all calculations independent of the different approximations to

$\varepsilon(q,\omega)$. Possible consequences of this inconsistency are examined with an approximate version of their semi-analytical LFC absorption model.

The LFC dielectric function in Vinko *et al* is replaced by the Hubbard approximation modified to satisfy the compressibility sum rule [4,5]. The Hubbard approximation is not only easier to compute but earlier work already obtained $R_c = 0.71 Å$ when fitting the Fermi surface eigenvalues with this dielectric function [4]. In contrast, fitting the Fermi eigenvalues with the RPA dielectric function yields $R_c = 0.6 Å$ [1]. Clearly, R_c it is not independent of the dielectric function in Eq. (2).

The thermally averaged electron-ion collision frequency is computed in the Born approximation [3] using the frequency dependent Hubbard dielectric function, but with the ion-ion structure factor set to unity. The ratio of two absorption cross-section calculations for cold, solid density Al using the present model with $R_c = 0.6 Å$ and $R_c = 0.71 Å$ is displayed in Fig. 1. The plot shows significant sensitivity of the photon absorption model to the free parameter R_c. The larger value of R_c comes from the consistently constrained pseudo-potential with the Hubbard approximation while the smaller value is inconsistent since it was obtained using the RPA result. Hence, a consistent treatment may affect the conclusions by Vinko *et al* regarding their LFC calculations.

It is stressed that the empirical pseudo-potential model constrained by Fermi surface eigenvalues has successfully reproduce properties of cold Al [4]. On the other hand, the electrical conductivity (a quantity directly related to the photon absorption [6]) of molten Al was found to be in poor agreement with experiments, which was attributed to limitations of the weak-scattering approximation rather than problems with the pseudo-potential method [4]. Furthermore, it is not obvious that an approach designed to describe quasi-particle behavior near the Fermi surface [4] can be extrapolated to calculate properties involving particle excitations involving several times the Fermi energy where the quasi-particle description rapidly becomes invalid. These comments suggest that the Vinko et al [1] approach would not be expected to reproduce reliably the XUV absorption properties of simple metals.

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References

[1] S.M. Vinko *et al*, *HEDP* **5** (2009) 124.

[2] A. Ron & N. Tzoar, *Phys. Rev.* **131** (1963) 12

[3] C.A. Iglesias, *HEDP*, in press

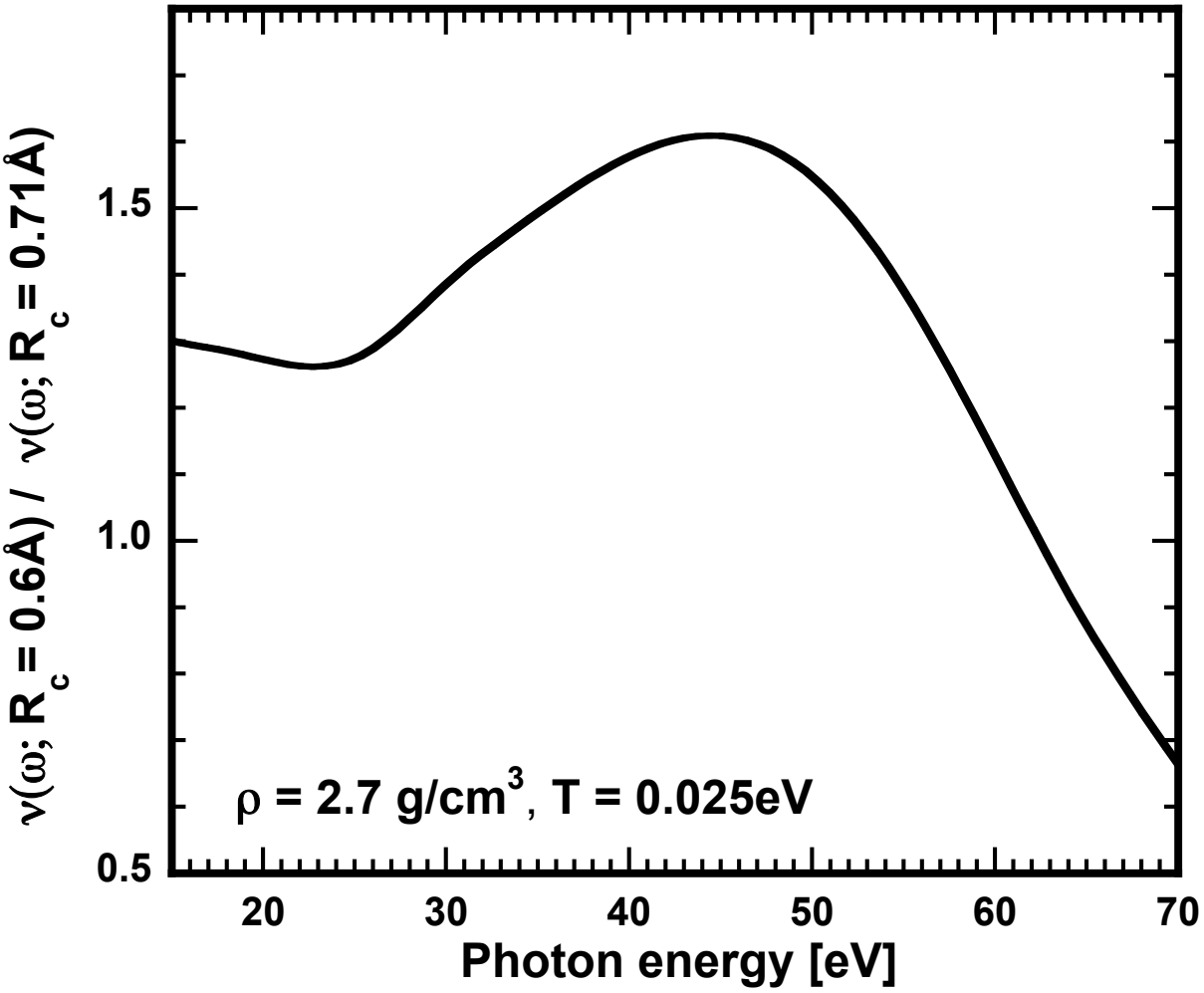
[4] A.P. Horsfield & N.W. Ashcroft, *J.Phys. Condens. Matter* **5** (1993) 3925

[5] J. Hubbard, *Proc.Roy.Soc.* **A243** (1957) 336

[6] S. Mazevet *et al*, *Phys. Rev.* **E71**, 016409(2005)

Figure Captions

Fig. 1 Ratio of thermally averaged electron-ion collision frequency for cold, solid density Al using present model with $R_c = 0.6\,\mathring{A}$ and $R_c = 0.71\,\mathring{A}$.



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